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published in

Modern Methods and Algorithms of Quantum Chemistry,
J. Grotendorst (Ed.), John von Neumann Institute for Computing, Jülich, NIC Series, Vol. **2**, ISBN 3-00-005746-3, p. 37, 2000.

http://www.fz-juelich.de/nic-series/

Ab initio investigation of the ground state of C_3H^-: Potential energy function and rovibrational spectrum

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Neutral unsaturated carbon chains and their ions have been the subject of much recent interest owing to their potential role in the chemistry of the interstellar medium. The detection of spectra for such species and their interpretation is greatly aided by simultaneous theoretical studies.

This poster presents a six−dimensional *ab initio* potential energy surface (PES) for the ground singlet state of C_3H^- generated using the CCSD(T) method and the aug−cc−pVQZ basis set. In agreement with previous studies, the global potential minimum corresponds to a cyclic isomer (C_{2v} , R_{CC}=1.380 Å, R_{CC}=1.380 Å, R_{CH}=1.083 Å, $C\hat{C}H$ =46.9°) and a local minimum is also located, about 2500 cm^{-1} higher in energy, corresponding to a planar trans bent isomer (C_s , R_{CC}=1.363 Å, R_{CC}=1.289 Å, R_{CH}=1.110 Å, $C\hat{C}C$ =109.2°, $C\hat{C}H$ =171.7°). The PES, represented by a fitted analytical form in the region of the two minima, is used in variational calculations to determine anharmonic rovibrational term values for both isomers and their deuterated analogues. Rotational, centrifugal distortion and vibration−rotation constants are also evaluated.